NuTroNS 1:
Joint EC-IAEA Nuclear Science Training Course on Nuclear Science with NUCLEONICA, Monaco, 12-15th Oct. 2010

European Commission Joint Research Centre

IAEA.org International Atomic Energy Agency

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NUCLEONICA:
Decay Engine

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Some theory…

Launching Decay Engine…

Performing calculation with default settings…

Exploring calculation results…

Selecting options…

Plotting results…

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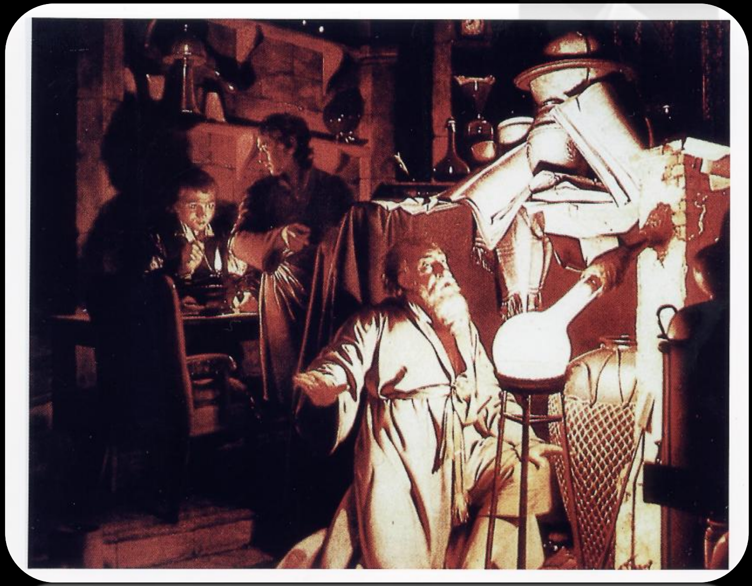
Modern Alchemy: Discovery of transmutation, (Soddy 1901)

In 1901, twenty-four year-old chemist Frederick Soddy and Ernest Rutherford were attempting to identify a mysterious gas that wafted from samples of radioactive thorium oxide. They suspected that this gas—they called it an “emanation”—held a key to the recently discovered phenomenon of radioactivity. Soddy had passed the puzzling gas over a series of powerful chemical reagents, heated white-hot. When no reactions took place, he came to a startling realization. As he told his biographer many years later….

´I remember quite well standing there transfixed as though stunned by the colossal import of the thing and blurting out- or so it seemed at the time: “Rutherford, this is transmutation: the thorium is disintegrating and transmuting itself into argon gas“. Rutherford‘s reply was typically aware of more practical implications,“For Mike‘s sake, Soddy, don‘t call it *transmutation*. They‘ll have our our heads off as alchemists“`

*quoted in *Pioneer*, pp 83-84

Frederic Soddy



Joseph Wright (1734-1797)

Simple radioactive decay..

Basic equation first identified by Rutherford

$$dQ/dt = -kQ \qquad (1)$$

Q is the number of atoms, k is the decay constant (probability per unit time that a nucleus will decay):

$$k = \ln 2 / \tau$$

where τ is the half-live. Solution of Eq.1...

$$Q(t) = Q(0)\, e^{-kt} \quad \text{or} \quad Q(t) = Q(0)\, 2^{-t/\tau}$$

Activity..

$$A(t) = k\, Q(t)$$

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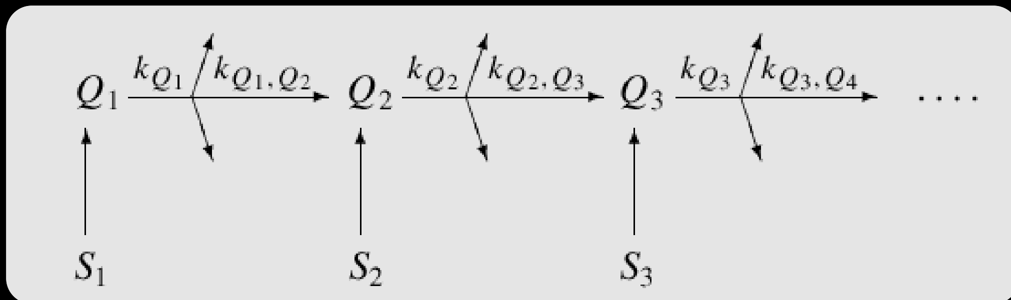
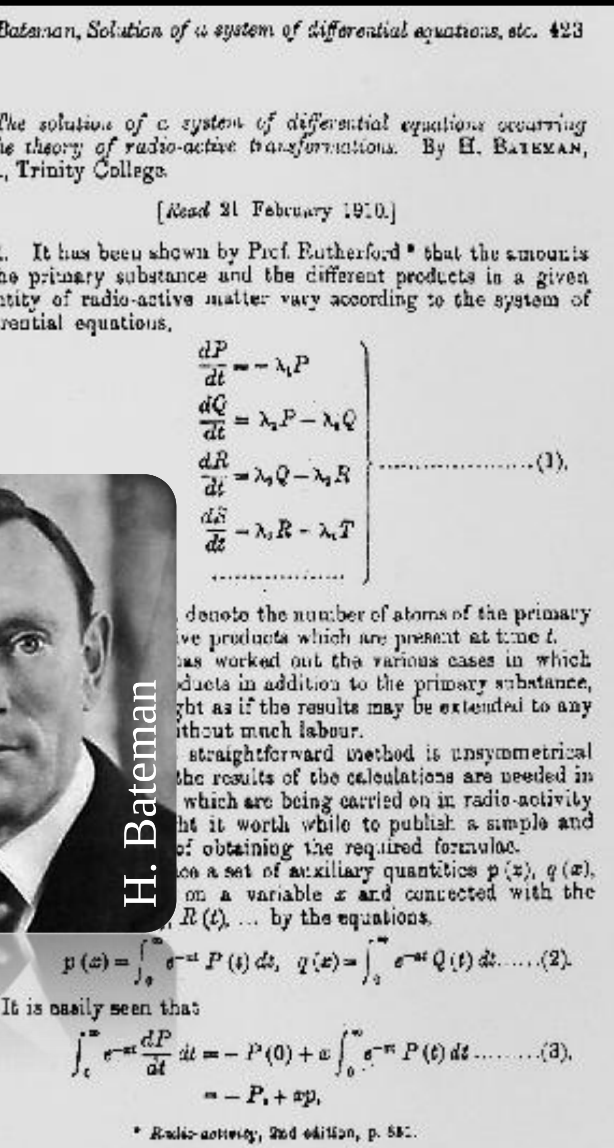
Successive radioactive decay with branching and source terms



The differential equations governing the above processes:

$$\mathrm{d}Q_1/\mathrm{d}t = S_1 - k_{Q_1} \cdot Q_1 \,,$$
$$\mathrm{d}Q_2/\mathrm{d}t = S_2 + k_{Q_1,Q_2} \cdot Q_1 - k_{Q_2} \cdot Q_2 \,,$$
$$\mathrm{d}Q_i/\mathrm{d}t = S_i + k_{Q_{i-1},Q_i} \cdot Q_{i-1} - k_{Q_i} \cdot Q_i \,,$$
$$\mathrm{d}Q_\mathrm{n}/\mathrm{d}t = S_\mathrm{n} + k_{Q_{\mathrm{n}-1},Q_\mathrm{n}} \cdot Q_{\mathrm{n}-1} - k_{Q_\mathrm{n}} \cdot Q_i \,,$$


Mr Bateman, Solution of a system of differential equations, etc. 423

The solution of a system of differential equations occurring in the theory of radio-active transformations. By H. BATEMAN, M.A., Trinity College.

[*Read* 21 February 1910.]

1. It has been shown by Prof. Rutherford* that the amounts of the primary substance and the different products in a given quantity of radio-active matter vary according to the system of differential equations,

$$\frac{dP}{dt} = -\lambda_1 P$$
$$\frac{dQ}{dt} = \lambda_1 P - \lambda_2 Q$$
$$\frac{dR}{dt} = \lambda_2 Q - \lambda_3 R \quad \text{.....................(1)}$$
$$\frac{dS}{dt} = \lambda_3 R - \lambda_4 T$$
....

... denote the number of atoms of the primary ... ive products which are present at time t.
... has worked out the various cases in which ... ducts in addition to the primary substance, ... ght as if the results may be extended to any ... ithout much labour.
... straightforward method is unsymmetrical ... the results of the calculations are needed in ... which are being carried on in radio-activity ... ht it worth while to publish a simple and ... of obtaining the required formulae.
... ce a set of auxiliary quantities $p(x)$, $q(x)$, ... on a variable x and connected with the ... $R(t)$, ... by the equations

$$p(x) = \int_0^\infty e^{-xt} P(t)\, dt, \quad q(x) = \int_0^\infty e^{-xt} Q(t)\, dt \text{ .....(2).}$$

It is easily seen that

$$\int_0^\infty e^{-xt} \frac{dP}{dt}\, dt = -P(0) + x\int_0^\infty e^{-xt} P(t)\, dt \text{ ....(3),}$$
$$= -P_0 + xp,$$

* Radio-activity, 2nd edition, p. 33[illegible].

Exact solution:

$$Q_{\mathrm{n}}(t) = \sum_{i=1}^{i=n} \left[\left(\prod_{j=1}^{j=n-1} k_{j,j+1} \right) \times \sum_{j=i}^{j=n} \left(\frac{Q_i(0)\,\mathrm{e}^{-k_j t}}{\prod\limits_{\substack{p=i \\ p\neq j}}^{n} (k_p - k_j)} + \frac{S_i\left(1-\mathrm{e}^{-k_j t}\right)}{k_j \prod\limits_{\substack{p=i \\ p\neq j}}^{n} (k_p - k_j)} \right) \right]$$

$$Q_{\mathrm{n}}(t) = \prod_{j=1}^{j=n-1} k_{j,j+1} \sum_{j=i}^{j=n} \frac{Q_i(0)\,\mathrm{e}^{-k_j t}}{\prod\limits_{\substack{p=i \\ p\neq j}}^{n} (k_p - k_j)}$$

First few terms...

$$Q_1 = Q_1(0)\,\mathrm{e}^{-k_1 t}$$

$$Q_2 = k_{1,2} \left\{ \frac{Q_1(0)\,\mathrm{e}^{-k_1 t}}{k_2 - k_1} + \frac{Q_1(0)\,\mathrm{e}^{-k_2 t}}{k_1 - k_2} \right\}$$

$$Q_3 = k_{1,2}k_{2,3} \left\{ \frac{Q_1(0)\,e^{-k_1 t}}{(k_2 - k_1)(k_3 - k_1)} + \frac{Q_1(0)\,\mathrm{e}^{-k_2 t}}{(k_1 - k_2)(k_3 - k_2)} + \frac{Q_1(0)\,\mathrm{e}^{-k_3 t}}{(k_1 - k_3)(k_2 - k_3)} \right\}$$

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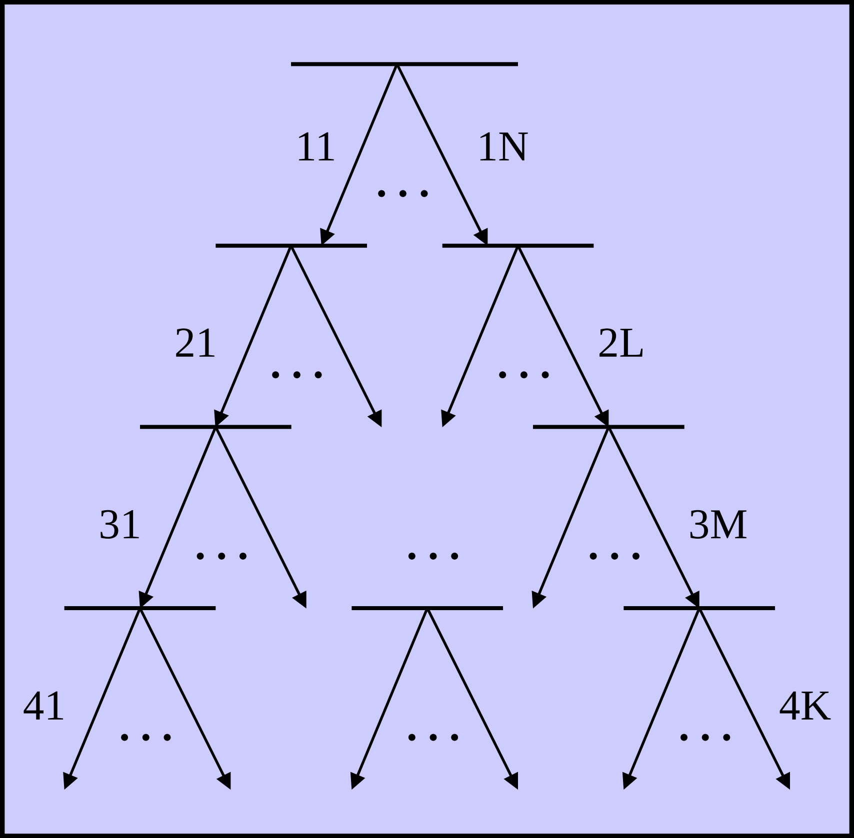
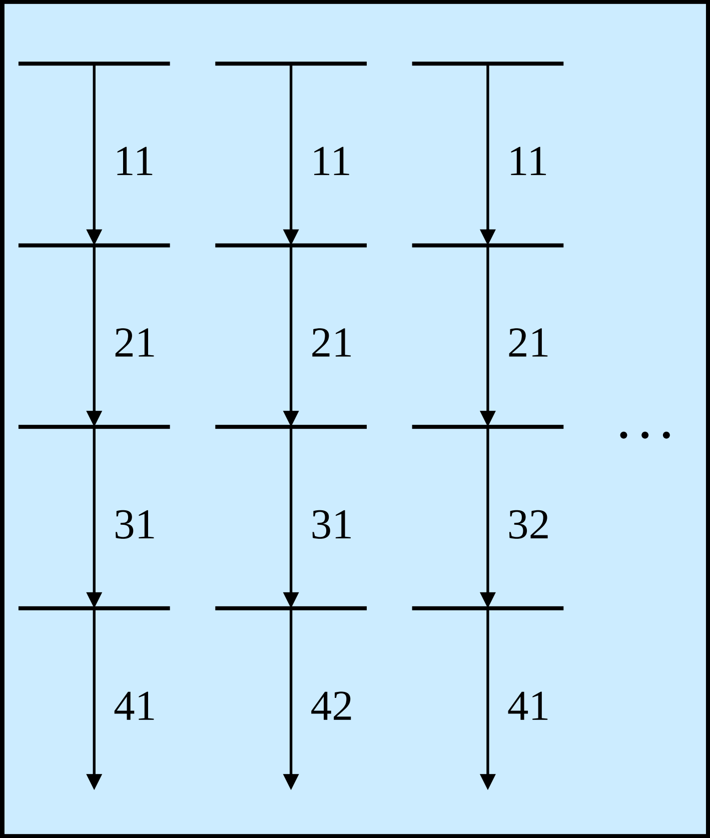
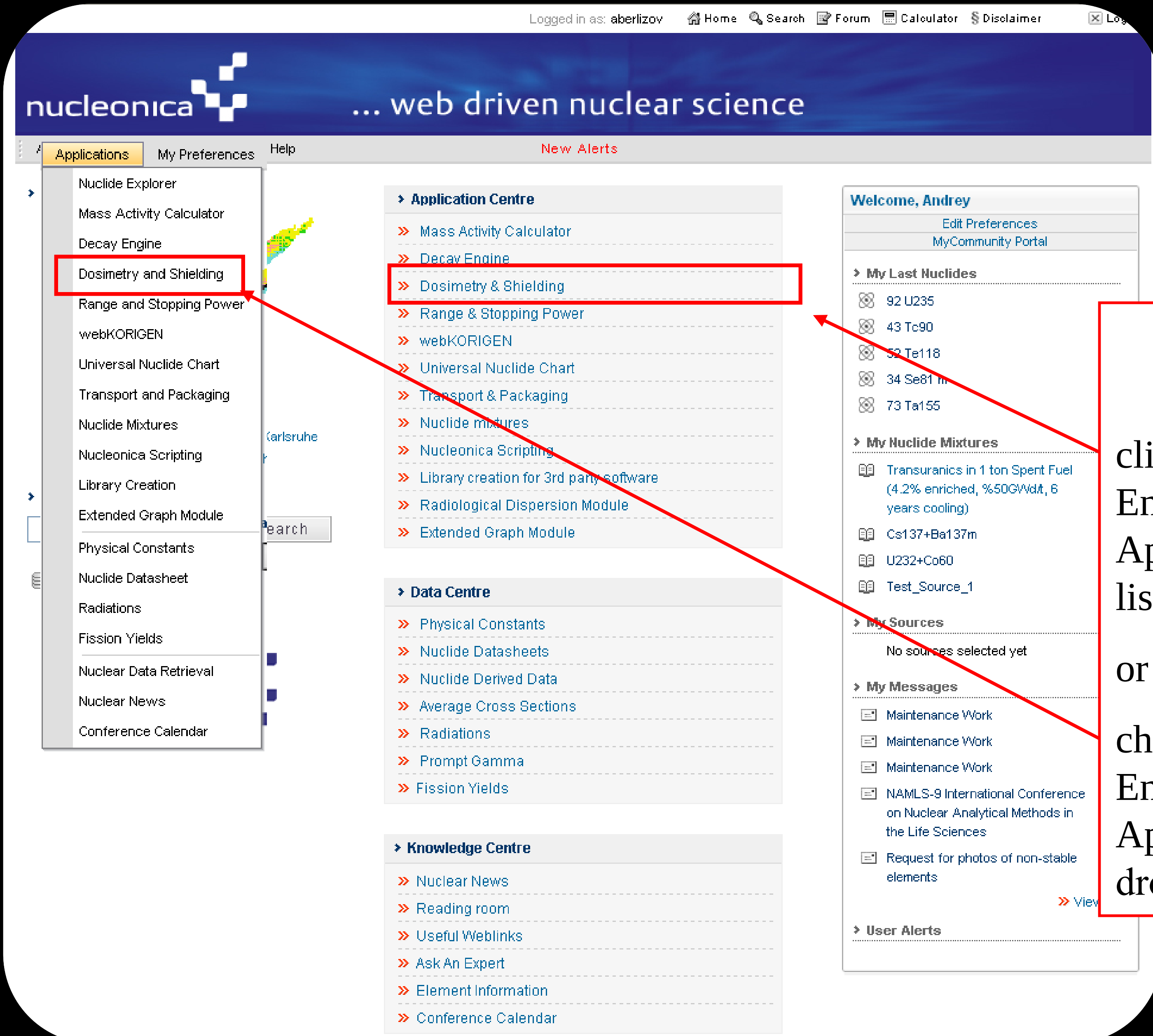
Decay Tree



Linear Chains



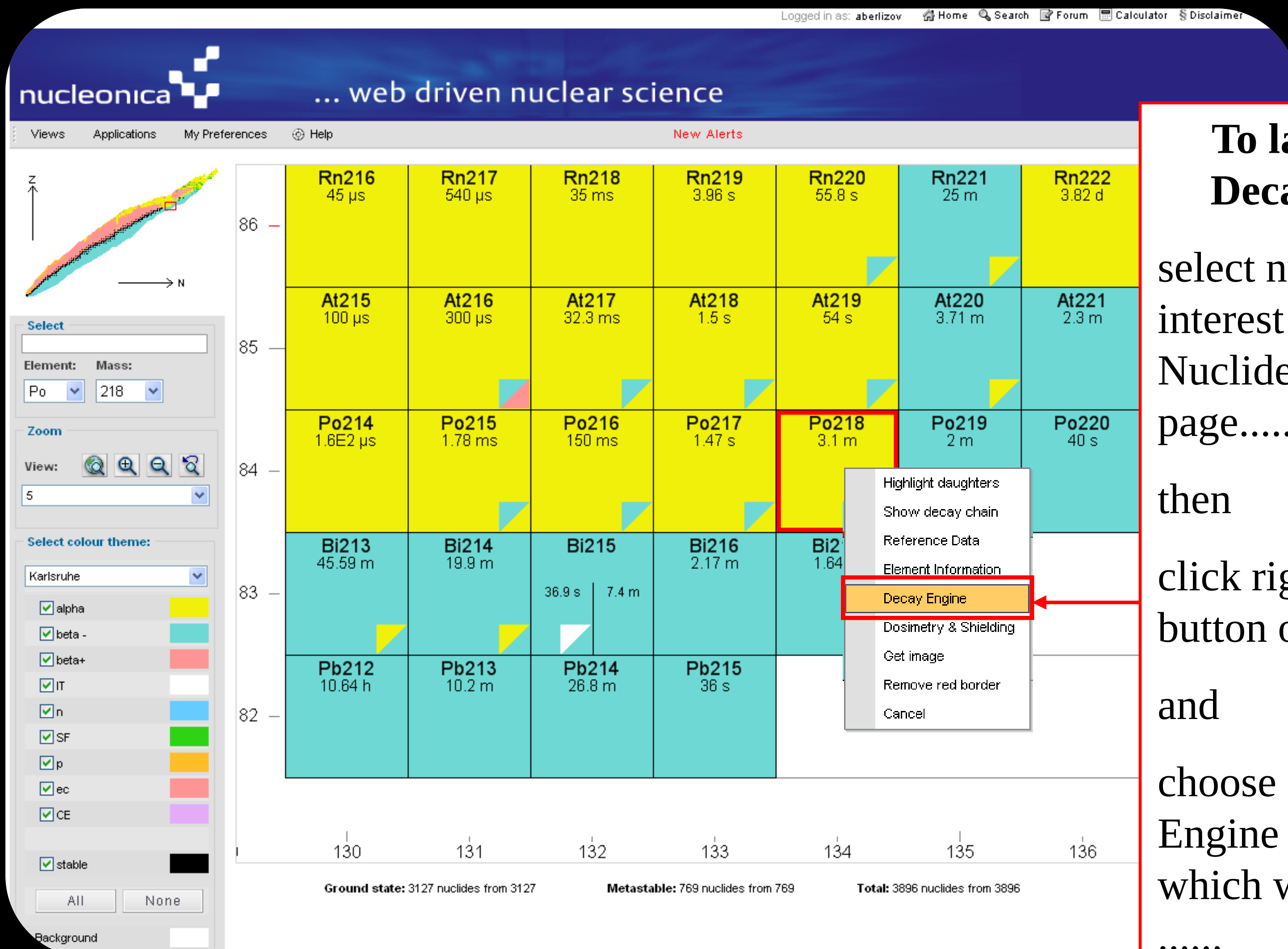


To launch the Decay Engine

click on Decay Engine in the Application Center list......

or

choose Decay Engine from the Applications dropdown list….



To launch the Decay Engine

select nuclide of interest in the Nuclide Explorer page......

then

click right mouse button over it ......

and

choose Decay Engine from the list, which will appear ......

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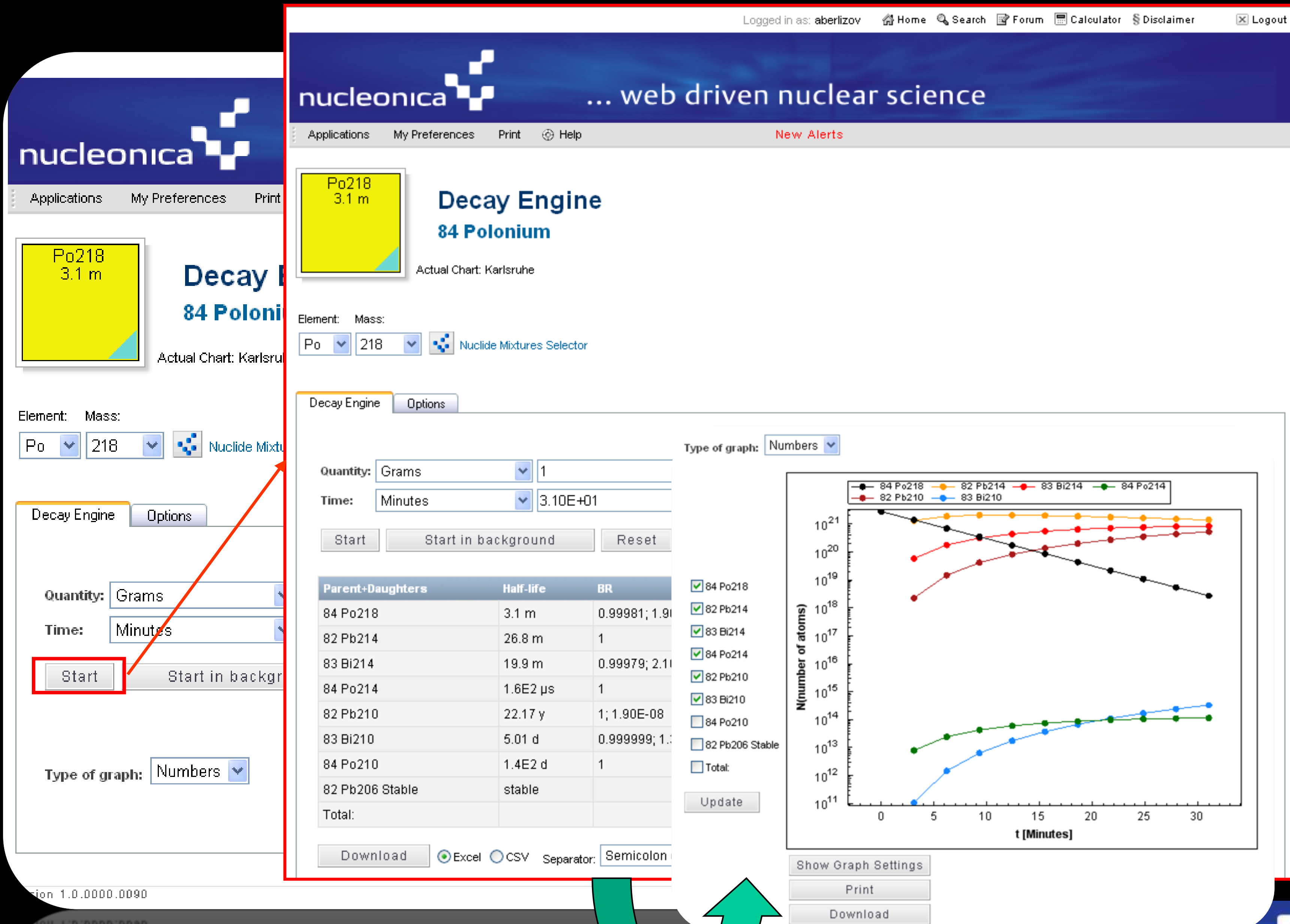
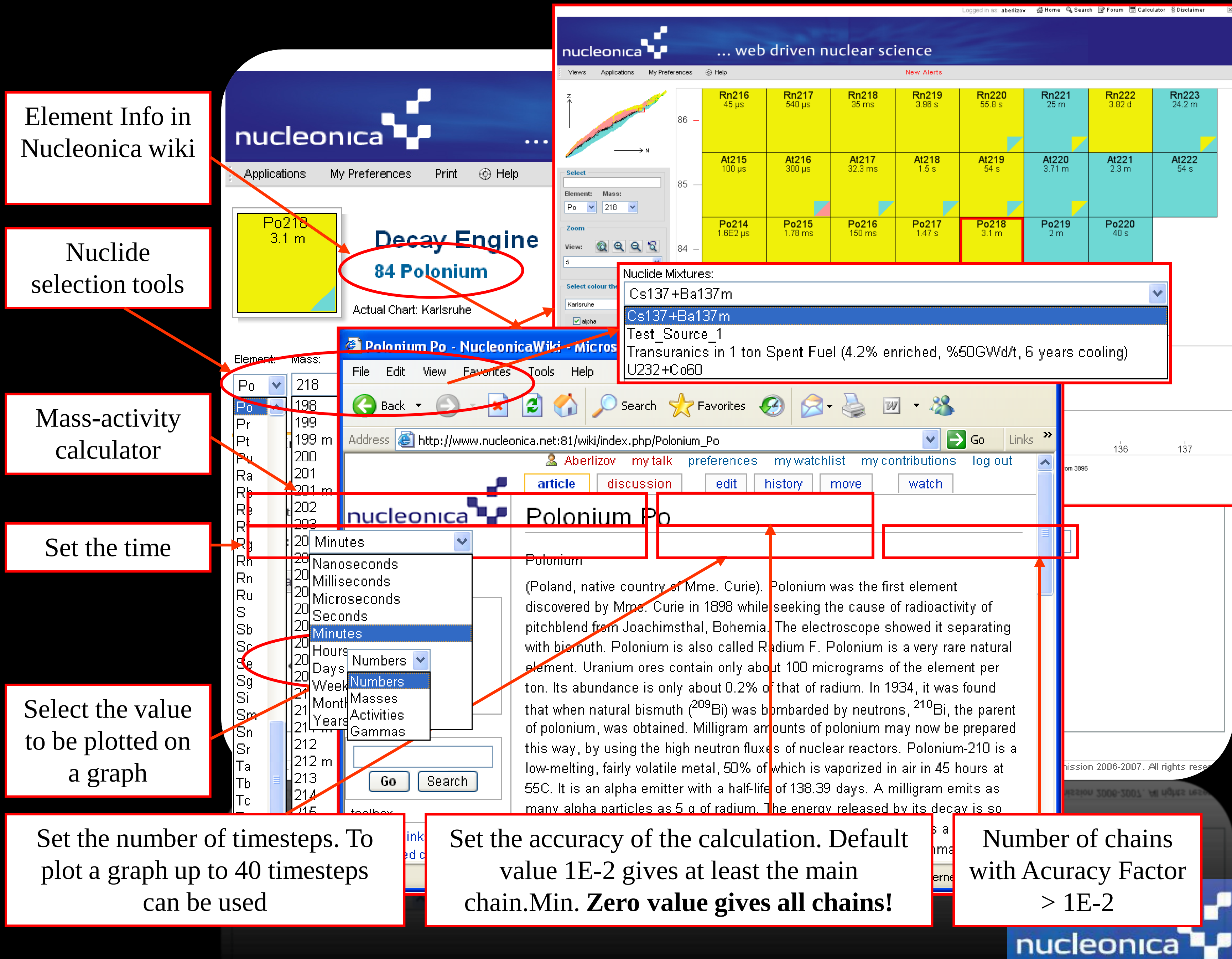


Start a calculation using default values....



Element Info in Nucleonica wiki
Nuclide selection tools
Mass-activity calculator
Set the time
Select the value to be plotted on a graph
Set the number of timesteps. To plot a graph up to 40 timesteps can be used
Set the accuracy of the calculation. Default value 1E-2 gives at least the main chain.Min. **Zero value gives all chains!**
Number of chains with Acuracy Factor > 1E-2
nucleonica ... web driven nuclear science
Decay Engine
84 Polonium
Actual Chart: Karlsruhe
Po218 3.1 m
Element: Mass:
Po 218
Nuclide Mixtures:
Cs137+Ba137m
Test_Source_1
Transuranics in 1 ton Spent Fuel (4.2% enriched, %50GWd/t, 6 years cooling)
U232+Co60
Polonium Po - NucleonicaWiki
http://www.nucleonica.net:81/wiki/index.php/Polonium_Po
Polonium Po
Minutes
Nanoseconds
Milliseconds
Microseconds
Seconds
Minutes
Hours
Days
Numbers
Masses
Activities
Gammas
Go Search

Po218
3.1 m

Decay Engine

84 Polonium

Actual Chart: Karlsruhe

1
84 Po218 2.71E+18
82 Pb214 1.40E+21
83 Bi214 8.35E+20
84 Po214 1.15E+14
82 Pb210 5.25E+20
83 Bi210 3.28E+14
84 Po210 2.39E+11
82 Pb206 Stable 3.21E+06
Prod = 1.00E+00
Total = 2.76E+21

2
84 Po218 2.71E+18
82 Pb214 1.40E+21
83 Bi214 8.35E+20
81 Tl210 1.12E+16
82 Pb210 9.90E+16
83 Bi210 5.79E+10
84 Po210 3.98E+07
82 Pb206 Stable 4.23E+02
Prod = 2.10E-04
Total = 2.24E+21

3
84 Po218 2.71E+18
85 At218 4.19E+12
83 Bi214 2.11E+17
84 Po214 2.89E+10
82 Pb210 3.13E+17
83 Bi210 2.90E+11
84 Po210 2.76E+08
82 Pb206 Stable 6.41E+03
Prod = 1.90E-04
Total = 3.23E+18

4
84 Po218 2.71E+18
82 Pb214 1.40E+21
83 Bi214 8.35E+20
82 Pb210 1.57E+16
83 Bi210 9.85E+09
84 Po210 7.17E+06
82 Pb206 Stable 1.17E+02
Prod = 3.00E-05
Total = 2.24E+21

5
84 Po218 2.71E+18
82 Pb214 1.40E+21
83 Bi214 8.35E+20
84 Po214 1.15E+14
82 Pb210 5.25E+20
83 Bi210 3.28E+14
81 Tl206 1.50E+05
82 Pb206 Stable 1.65E+05
Prod = 1.32E-06
Total = 2.76E+21

6
84 Po218 2.71E+18
85 At218 4.19E+12
86 Rn218 9.77E+07
84 Po214 4.57E+05
82 Pb210 5.24E+14
83 Bi210 8.25E+08
84 Po210 1.08E+06
82 Pb206 Stable 3.39E+01
Prod = 1.90E-07
Total = 2.71E+18

7
84 Po218 2.71E+18
85 At218 4.19E+12
83 Bi214 2.11E+17
81 Tl210 3.09E+12
82 Pb210 6.26E+13
83 Bi210 5.40E+07
84 Po210 4.82E+04
82 Pb206 Stable 1.11E+00
Prod = 3.99E-08
Total = 2.92E+18

8
84 Po218 2.71E+18
82 Pb214 1.40E+21
83 Bi214 8.35E+20
84 Po214 1.15E+14
82 Pb210 5.25E+20
80 Hg206 3.63E+06
81 Tl206 1.19E+06
82 Pb206 Stable 1.42E+06
Prod = 1.90E-08
Total = 2.76E+21

9
84 Po218 2.71E+18
82 Pb214 1.40E+21
83 Bi214 8.35E+20
81 Tl210 1.12E+16
82 Pb209 6.69E+12
83 Bi209 2.36E+11
81 Tl205 Stable 0.00E+00
Prod = 1.47E-08
Total = 2.24E+21

10
84 Po218 2.71E+18
85 At218 4.19E+12
83 Bi214 2.11E+17
82 Pb210 9.39E+12
83 Bi210 8.71E+06
84 Po210 8.28E+03
82 Pb206 Stable 0.00E+00
Prod = 5.69E-09
Total = 2.92E+18

Accuracy Factor: 0

Number of timesteps: 10

Number of chains: 23

Reset | Show Details | Create Nuclide Mixture

	Decay	N(atoms)	M(g)	A(Bq)
		2.76E+21	9.78E-01	1.58E+18
	ß-	1.40E+21	4.97E-01	6.03E+17
99979; 2.10E-04; 3.00E-05	ß-; α; ß-,α	8.36E+20	2.97E-01	4.85E+17
	α	1.15E+14	4.07E-08	4.85E+17
99981; 1.90E-04	α; ß-	2.71E+18	9.81E-04	1.01E+16
99993; 7.00E-05	ß-; ß-,n	1.12E+16	3.91E-06	9.97E+13
999; 1.00E-03	α; ß-	4.19E+12	1.52E-09	1.94E+12
1.90E-08	ß-; α	5.25E+20	1.83E-01	5.20E+11
	α	9.77E+07	3.54E-14	1.94E+09
999999; 1.32E-06	ß-; α	3.29E+14	1.15E-07	5.26E+08
	ß-	6.70E+12	2.32E-09	3.96E+08
	α	2.39E+11	8.35E-11	1.39E+04
	ß-	3.64E+06	1.24E-15	5.16E+03
	ß-	1.34E+06	4.58E-16	3.68E+03
	α	2.36E+11	8.21E-11	2.73E-16
		4.80E+06	1.64E-15	0
		0	0	0

Semicolon (";") ☑ Use field qualifier (")

Click on the column title to arrange the data in ascending /descending order on the parameter chosen

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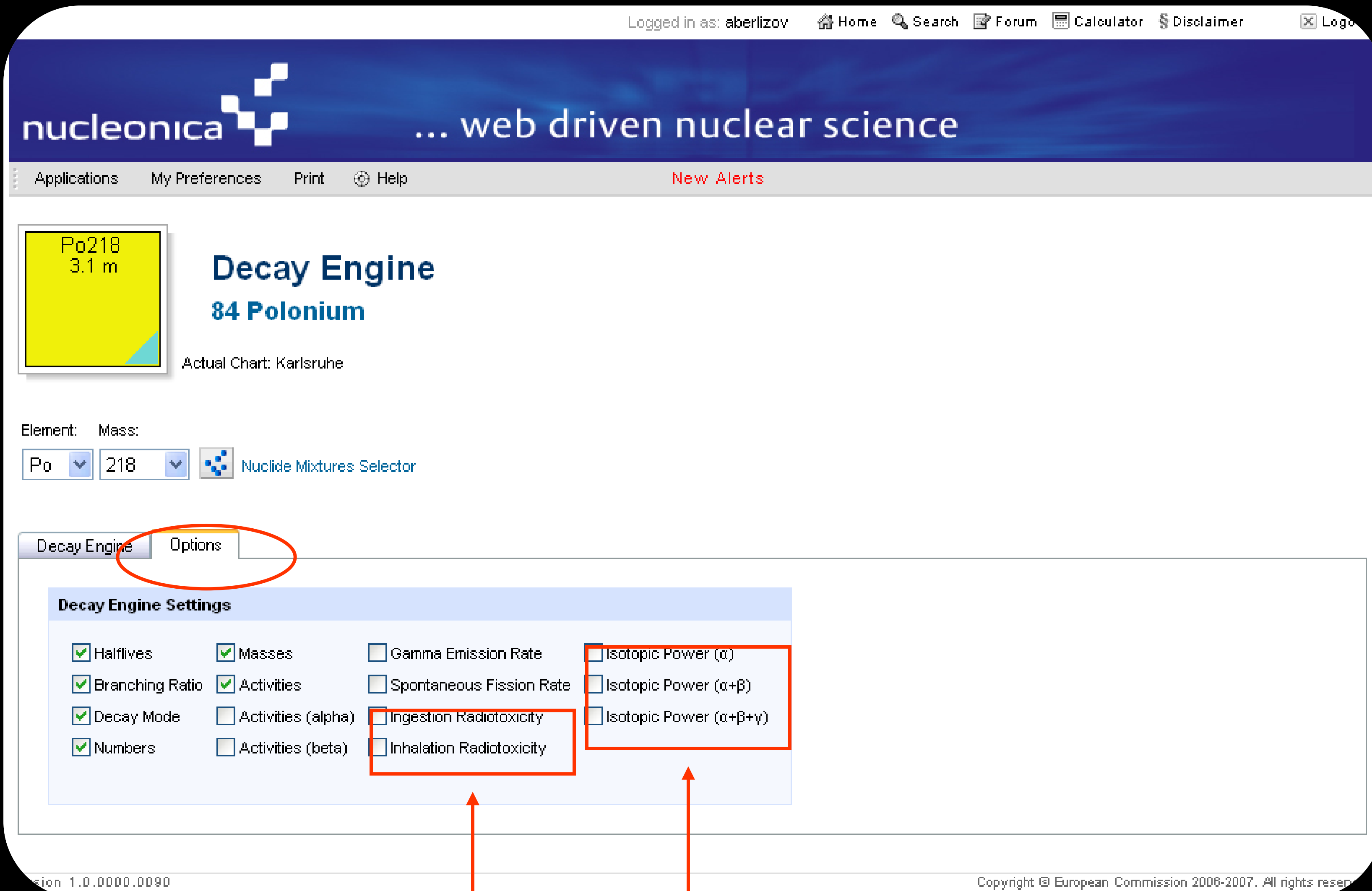
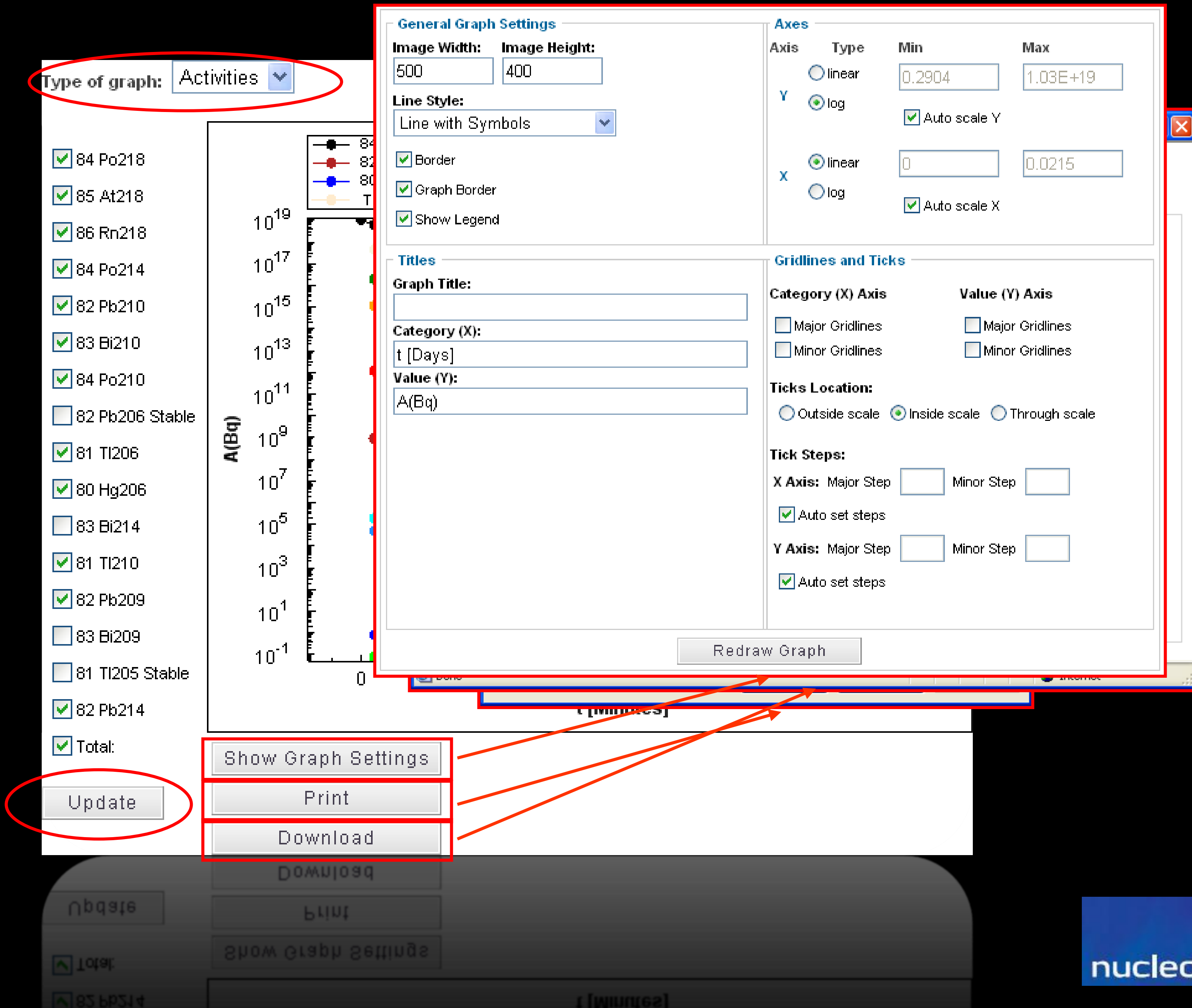
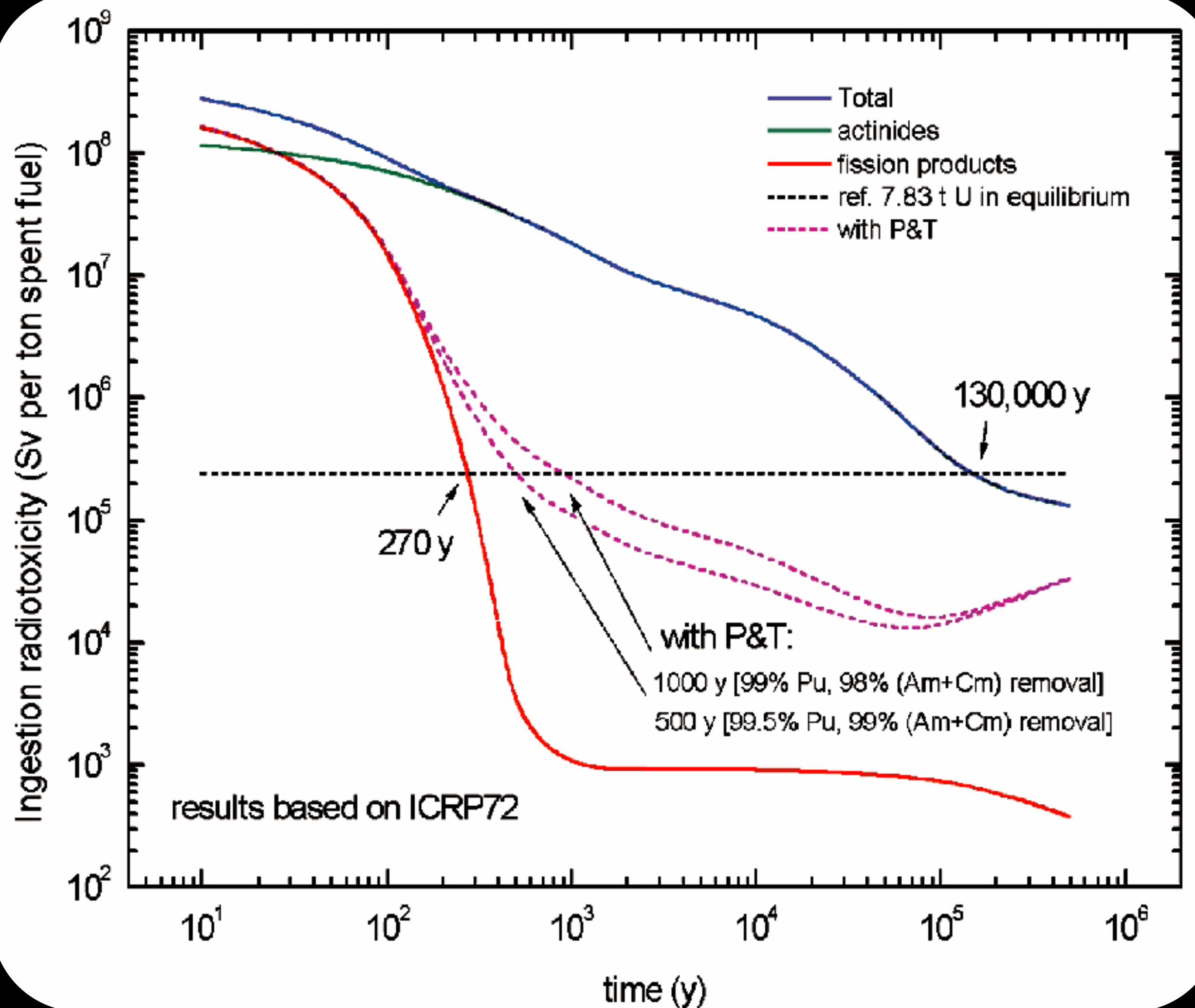


Radiotoxicity (Sv) = Activity · *e*(50), where e(50) - effective dose coefficient, which accounts for radiation and tissue weighting factors, metabolic and biokinetic information.

the heat generated per unit time by the decay radiations (W)


Type of graph: Activities
84 Po218
85 At218
86 Rn218
84 Po214
82 Pb210
83 Bi210
84 Po210
82 Pb206 Stable
81 Tl206
80 Hg206
83 Bi214
81 Tl210
82 Pb209
83 Bi209
81 Tl205 Stable
82 Pb214
Total:
Update
Show Graph Settings
Print
Download
A(Bq)
General Graph Settings
Image Width: 500
Image Height: 400
Line Style: Line with Symbols
Border
Graph Border
Show Legend
Axes
Axis Type Min Max
Y linear log 0.2904 1.03E+19 Auto scale Y
X linear log 0 0.0215 Auto scale X
Titles
Graph Title:
Category (X): t [Days]
Value (Y): A(Bq)
Gridlines and Ticks
Category (X) Axis
Value (Y) Axis
Major Gridlines
Minor Gridlines
Ticks Location:
Outside scale
Inside scale
Through scale
Tick Steps:
X Axis: Major Step Minor Step
Auto set steps
Y Axis: Major Step Minor Step
Auto set steps
Redraw Graph



Ingestion radiotoxicity (Sv per ton spent fuel)
time (y)
Total
actinides
fission products
ref. 7.83 t U in equilibrium
with P&T
130,000 y
270 y
with P&T:
1000 y [99% Pu, 98% (Am+Cm) removal]
500 y [99.5% Pu, 99% (Am+Cm) removal]
results based on ICRP72

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Some theory…

Launching Decay Engine…

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Plotting results…

Thanks!

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